Strongly consistent model selections for densities

Gérard Biau, Benoît Cadre, Luc Devroye, Laszlo Gyorfi

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Gérard Biau * Benoît Cadre * Luc Devroye †
László Györfi ‡

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Abstract

Let f be an unknown multivariate density belonging to a set of densities $\mathcal{F}_{k^*}$ of finite associated Vapnik-Chervonenkis dimension, where the complexity k^* is unknown, and $\mathcal{F}_k \subset \mathcal{F}_{k+1}$ for all k. Given an i.i.d. sample of size n drawn from f, this article presents a density estimate $\hat{f}_{K_n}$ yielding almost sure convergence of the estimated complexity K_n to the true but unknown k^*, and with the property $\mathbf{E}\{\int |\hat{f}_{K_n} - f|\} = \mathrm{O}(1/\sqrt{n})$. The methodology is inspired by the combinatorial tools developed in Devroye and Lugosi [8] and it includes a wide range of density models, such as mixture models and exponential families.

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*Institut de Mathématiques et de Modélisation de Montpellier – UMR CNRS 5149, Equipe de Probabilités et Statistique, Université Montpellier II, CC 051 – Place Eugène Bataillon, 34095 Montpellier Cedex 5, France.
e-mail: biau@math.univ-montp2.fr, cadre@math.univ-montp2.fr .
Corresponding author: Gérard Biau.

†School of Computer Science, McGill University, Montreal, QC H3A 2K6, Canada.
e-mail: luc@cs.mcgill.ca .

‡Department of Computer Science and Information Theory, Budapest University of Technology and Economics, H-1521 Stoczek u. 2, Budapest, Hungary.
e-mail: gyorfi@szit.bme.hu .

1 Introduction

Let $(\mathcal{F}_k)_{k\geq 1}$ be a sequence of nested parametric models of density functions on $\mathbb{R}^d$. Define

$$\mathcal{F} = \bigcup_{k\geq 1} \mathcal{F}_k.$$

In the union above, $\mathcal{F}_k$ denotes, for each fixed $k \geq 1$, a given class of densities parametrized by one or more parameters, and such that $\mathcal{F}_k \subset \mathcal{F}_{k+1}$ for all k. Typically, $\mathcal{F}_k$ may be the class of all mixtures of k Gaussian densities on $\mathbb{R}^d$, but many other nested models are possible, see below. In the present paper, we consider the general problem of estimating a density f which belongs to $\mathcal{F}$. Formally, we let the complexity associated with f be defined as

$$k^* = \min\{k \geq 1 : f \in \mathcal{F}_k\}.$$

Clearly, as it is supposed that $f \in \mathcal{F}$, we have $k^* < \infty$. Thus k^* just represents the index of the most parsimonious model for f. Given an i.i.d. random sample $X_1, \ldots, X_n$ drawn from f, this article presents a density estimate $\hat{f}_{K_n}$ yielding almost sure convergence of the estimated complexity K_n to the true but unknown k^*, and with the property that $\mathbf{E}\{\int |\hat{f}_{K_n} - f|\} = \mathrm{O}(1/\sqrt{n})$. Thus, we show how to pick a model complexity and a density from the given model, and still guarantee an $\mathrm{O}(1/\sqrt{n})$ rate of convergence for the expected error, just as if we had been given the model complexity beforehand. The strongly consistent estimate K_n is obtained by minimizing the L_1 error between candidate models and the standard histogram estimate. Based on this estimate, the model parameters are selected using the general combinatorial tools developed in Devroye and Lugosi [8]. Our methodology is close in spirit to Biau and Devroye [1], [2], who use a penalized combinatorial criterion to select a density from a nested sequence of models. However, these authors do not consider the estimation of the complexity parameter k^*, and they employ a penalty depending on a sequence of arbitrary weights, which renders the method difficult to implement. In contrast, the selection procedure presented in the present paper does not rely on any arbitrary penalty choice, and it seems therefore more tractable.

The paper is organized as follows. In section 2, we present our new histogram-based estimate K_n for the complexity k^* and show its strong consistency. In section 3, we develop our density estimation procedure and state its L_1-optimality. For the sake of clarity, proofs are gathered in section 4.

2 Complexity estimation

Without loss of generality, we assume that the sample of independent random vectors distributed according to the probability measure μ with density f is of even size $2n$. Let μ_{2n} be its empirical measure, *i.e.*, $\mu_{2n}(A) = \big(1/(2n)\big) \sum_{i=1}^{2n} \mathbf{1}_{\{X_i \in A\}}$. Split the sample into two subsamples: $X_1, \ldots, X_n$ and $\{X'_1, \ldots, X'_n\} = \{X_{n+1}, \ldots, X_{2n}\}$, and denote by μ_n and μ'_n the respective empirical measures. Let $\mathcal{P}_n = \{A_{n,j} : j \geq 1\}$ be a cubic partition of $\mathbb{R}^d$ with volume h_n^d. Introduce the statistic

$$d_{n,k} = \inf_{g \in \mathcal{F}_k} \sum_{A \in \mathcal{P}_n} \left| \int_A g - \mu_{2n}(A) \right|.$$

Roughly speaking, $d_{n,k}$ should be small if $f \in \mathcal{F}_k$. Consequently, let the threshold be

$$T_n = \sum_{A \in \mathcal{P}_n} |\mu_n(A) - \mu'_n(A)|.$$

Note that the statistic T_n has been introduced in Biau and Györfi [3], while its kernel version was studied in Cao and Lugosi [4]. We say that $d_{n,k}$ is small if it is smaller than T_n, so our estimate of k^* is

$$K_n = \min\{k \geq 1 : d_{n,k} \leq T_n\},$$

with the convention $\min\{\emptyset\} = \infty$. Clearly, the statistic $d_{n,k}$ is nonincreasing in k, so that this definition makes sense.

From a topological point of view, we will suppose throughout the paper that each $\mathcal{F}_k$ is a closed metric subspace of the space of all densities on $\mathbb{R}^d$ endowed with the weak convergence topology. In other words, for any sequence (g_n) in $\mathcal{F}_k$ satisfying

$$\lim_{n \to \infty} \int g_n(x)\varphi(x) \, \mathrm{d}x = \int g(x)\varphi(x) \, \mathrm{d}x$$

for every bounded, continuous real function φ, one has $g \in \mathcal{F}_k$. This requirement is not restrictive. For example, one may check that this prerequisite holds for the class $\mathcal{F}_k$ of all mixtures of k Gaussian densities on $\mathbb{R}^d$. In this case, each density f_k in $\mathcal{F}_k$ may be written as

$$f_k(x) = \sum_{i=1}^{k} \frac{p_i}{(2\pi)^{d/2}\sqrt{\det(\Sigma_i)}}\, e^{-\frac{1}{2}(x-m_i)^T \Sigma_i^{-1}(x-m_i)},$$

where $k < \infty$ is the mixture complexity, $p_i \geq 0$, $i = 1, \ldots, k$ are the mixture weights satisfying $\sum_{i=1}^{k} p_i = 1$, $m_1, \ldots, m_k$ are arbitrary elements of $\mathbb{R}^d$ and $\Sigma_1, \ldots, \Sigma_k$ are positive definite $d \times d$ matrices.

Methodologies for consistent estimation of a mixture distribution are well known. An enormous body of literature exists regarding the application, computational issues and theoretical aspects of mixture models when the number of components is known, but estimating the unknown number of components remains an area of intense research. The scope of application is vast, as mixture models are routinely employed across the entire diverse application range of statistics, including nearly all of the social and experimental sciences. Recent attempts at estimating the mixture density parameters and the number of mixture densities jointly are by Priebe [14], James, Priebe and Marchette [11], and Rogers, Marchette and Priebe [15]. For an updated list of references, we refer the reader to Biau and Devroye [2] and the discussion therein.

As another interesting collection of models, we might also consider the class of increasing exponential families. Each density f_k in an exponential family $\mathcal{F}_k$ may be written in the form

$$f_k(x) = c\alpha(\theta)\beta(x)e^{\sum_{i=1}^{k} \pi_i(\theta)\psi_i(x)},$$

where θ belongs to some parameter set Θ, $\psi_1, \ldots, \psi_k : \mathbb{R}^d \to \mathbb{R}$, $\beta : \mathbb{R}^d \to [0, \infty)$, $\alpha, \pi_1, \ldots, \pi_k : \Theta \to \mathbb{R}$ are fixed functions, and c is a normalization constant. Examples of exponential families include classes of Gaussian, gamma, beta, Rayleigh, and Maxwell densities. By allowing k to grow, this

model can become very rich and powerful.

Theorem 1. *Assume that, for each $k \geq 1$, $\mathcal{F}_k$ is closed with respect to the weak convergence topology. Choose $h_n = n^{-\delta}$ with $0 < \delta < 1/d$. Then there exists a positive constant κ, depending on f, such that*

$$\mathbf{P}\left\{K_n \neq k^*\right\} \leq \exp\left(-\kappa\, n^{d\delta}\right),$$

and consequently, almost surely,

$$K_n = k^*$$

for all n large enough.

3 Fast density estimate

In the same way as in Biau and Devroye [1], [2], based on the complexity estimation presented in the previous section, we consider a minimum distance type estimate. Using ideas from Yatracos [17], Devroye and Lugosi explore in [8] a new paradigm for the data-based or automatic selection of the free parameters of density estimates in general, so that the expected error is within a given constant multiple of the best possible error. To summarize in the present context, fix $k \geq 1$, and define a density estimate $\hat{f}_k$ in $\mathcal{F}_k$ as follows. First introduce the class of sets

$$\mathcal{A}_k = \left\{\{x : g_1(x) \geq g_2(x)\} : g_1, g_2 \in \mathcal{F}_k\right\}$$

($\mathcal{A}_k$ is the so-called Yatracos class associated with $\mathcal{F}_k$) and the goodness criterion for a density $g \in \mathcal{F}_k$:

$$\Delta_k(g) = \sup_{A \in \mathcal{A}_k} \left| \int_A g - \mu_{2n}(A) \right|.$$

Then the minimum distance estimate $\hat{f}_k$ is defined as any density estimate selected from among those densities $f_k \in \mathcal{F}_k$ with

$$\Delta_k(f_k) < \inf_{g \in \mathcal{F}_k} \Delta_k(g) + \frac{1}{2n}.$$

Note that the $1/(2n)$ term here is added to ensure the existence of such a density estimate. From now on, we let V_k be the Vapnik-Chervonenkis dimension of the class of sets $\mathcal{A}_k$ (Vapnik and Chervonenkis [16]).

Corollary 1. *Assume that V_{k^*} is finite. Then, under the conditions of Theorem 1, the minimum distance estimate $\hat{f}_{K_n}$ satisfies*

$$\mathbf{E}\left\{ \int |\hat{f}_{K_n} - f| \right\} = \mathrm{O}\left(\frac{1}{\sqrt{n}} \right). \tag{1}$$

PROOF. For the minimum distance estimate $\hat{f}_k$, we have (Devroye and Lugosi [8], Theorem 6.4, page 56)

$$\int |\hat{f}_k - f| \leq 3 \inf_{g \in \mathcal{F}_k} \int |g - f| + 4\Delta_k(f) + \frac{3}{2n}. \tag{2}$$

Since inequality (2) holds for every $k \geq 1$, it holds in particular for K_n. The corresponding minimum distance estimate, $\hat{f}_{K_n}$, is a natural candidate for the estimation of f. Clearly,

$$\int |\hat{f}_{K_n} - f| \leq \int |\hat{f}_{K^*} - f| \; \mathbf{1}_{\{K_n = k^*\}} + 2\, \mathbf{1}_{\{K_n \neq k^*\}}.$$

By inequality (2), we have, for all $n \geq 1$,

$$\int |\hat{f}_{K^*} - f| \leq 4\Delta_{K^*}(f) + \frac{3}{2n}.$$

Using Theorem 1, we deduce that

$$\mathbf{E}\left\{ \int |\hat{f}_{K_n} - f| \right\} \leq 4\mathbf{E}\left\{ \Delta_{k^*}(f) \right\} + \frac{3}{2n} + 2\exp\left(-\kappa\, n^{d\delta} \right), \tag{3}$$

where κ is the positive constant of Theorem 1. The uniform convergence of empirical measures as developed by Vapnik and Chervonenkis [16] can now be applied to density estimation via the term $\Delta_{k^*}(f)$. A standard inequality from empirical process theory (Dudley [9]) shows that if $\mathcal{A}_{k^*}$ has Vapnik-Chervonenkis dimension V_{k^*}, then

$$\mathbf{E}\left\{ \Delta_{k^*}(f) \right\} \leq C\sqrt{\frac{V_{k^*}}{n}}, \tag{4}$$

where C is a positive universal constant. Inequalities (3) and (4) then imply

$$\mathbf{E}\left\{ \int |\hat{f}_{K_n} - f| \right\} \leq 4C\sqrt{\frac{V_{k^*}}{n}} + \frac{3}{2n} + 2\exp\left(-\kappa\, n^{d\delta}\right).$$

■

As an illustration, consider the examples of section 2. It can be shown (see Devroye and Lugosi [8], Chapter 8) that $V_k = \mathrm{O}(k^4)$ for the univariate Gaussian mixtures with k components, and $V_k \leq k+1$ for the exponential families. Equality (1) is thus satisfied by a large collection of models.

It is strictly speaking not necessary that $V_k \to \infty$, although such situations are of little general interest. Indeed, if $\sup_{k\geq 1} V_k < \infty$, then the Vapnik-Chervonenkis dimension of the infinite union $\mathcal{F}$ is finite, and one could just apply the ordinary combinatorial method. However, in most situations of interest, the Vapnik-Chervonenkis dimension of $\mathcal{F}$ is infinite, and we cannot use the original combinatorial method. It is to correct this situation that we presented the two step procedure.

Observe also that the finiteness of the associated Vapnik-Chervonenkis dimension is only used at k^*. We thus allow this dimension to be infinite starting at any $k > k^*$. Considering a silly example, we could take as $\mathcal{F}_{k^*+1}$ the class of all densities. Then the $d_{n,k}$ value is zero at k^*+1, so the selected k is never more than k^*+1. But the method is clever enough to stop at k^*. If you stop at k^*+1, then the minimum distance estimate includes any density. So the penalty for overshooting is high.

We note that our model selection procedure is simpler than that of Biau and Devroye [1], since the projection over a cubic partition is easier than the projection over a Yatracos class. However, practically speaking, several questions need to be addressed, including that of the effective computation of the minimum distance estimate $\hat{f}_k$. To date, we do not know any method for its precise computation. Discretized methods and randomized methods that provide acceptable and computationally feasible approximation have

been used in the simulation study of Devroye [5]. However, those simulations only involve one-dimensional problems, and thus, much more work is needed. In fact, the exploration of the relationship between class complexity, computational complexity and approximation seems very interesting. One may follow the model of pattern recognition and machine learning, where these connections have been thoroughly studied.

Summarizing, we have thus shown, assuming that $f \in \mathcal{F}$, how to pick a mixture complexity and a density from the given mixture, and still guarantee an $O(1/\sqrt{n})$ rate of convergence for the expected error, just as if we had been given the mixture complexity beforehand. On the other hand, we realize that an important situation occurs when our infinite union is dense in the set of all densities, all Vapnik-Chervonenkis dimensions are finite, and the density is not in any $\mathcal{F}_k$. Note that T_n depends upon n and h_n in the standard way. Now, $d_{n,k}$ tends to zero with k, so we end up anyway with a finite K_n. As $d_{n,k}$ is below T_n by our selection criterion, it seems that we can have an error bound of the order of the bound for T_n. This would mean that we can in the worst case have a bound as for the classical histogram (because that is what T_n will give). We believe however that such results are beyond the scope of the present paper and we will deal with this problem elsewhere.

Remark 1. Recall that when the set $\{k \geq 1 : d_{n,k} \leq T_n\}$ is empty, we decide $K_n = \infty$ by convention. In this case, any choice in $\mathcal{F}$ for $\hat{f}_{K_n}$ will do. ■

Remark 2. For the actual density estimate, we could not avoid the projection over the Yatracos class. Thus, we could not decrease the computational complexity. It is an open problem whether simply the projection over a cubic partition is a proper density estimate. Note also that the histogram is only used to select k^*. The actual density estimate depends upon the Yatracos classes – the histogram is thrown away! This point is essential, as a histogram estimate cannot converge at the rate $O(1/\sqrt{n})$. So we have the

apparent paradox that a density estimate with a bad rate can be used to obtain – in two steps – a great rate! In a sense, the histogram is used to choose the complexity (or lack of smoothness) of another class of functions. The choice of the histogram's width, h_n, thus has a secondary effect. To stay within the limits of the theorem, one could easily replace h_n by one of the many data-dependent and automated bandwidths. Some of these are discussed or surveyed in Devroye and Györfi [6] and Devroye and Lugosi [8].

Interestingly, in the second step, and under some conditions, just the projection of another, non-consistent (asymptotically biased) histogram can result in a density estimate with good rate, too. With this respect, denote by $\xi_{n,r}$ a histogram estimate constructed using the sample $X_1, \ldots, X_{2n}$ and a cubic partition $\{B_{r,j} : j \geq 1\}$ of $\mathbb{R}^d$ with volume r^d, and let $\pi_r(g)$ be the expectation of this histogram for the density g, that is

$$\pi_r(g)(x) = \frac{1}{r^d} \int_{B_r(x)} g,$$

where $B_r(x)$ is the cell of the partition containing x. Let the estimate $\tilde{f}_{n,r}$ be defined as

$$\tilde{f}_{n,r} = \arg\min_{g \in \mathcal{F}_{K_n}} \int |\pi_r(g) - \xi_{n,r}|.$$

Suppose moreover that the bin width r is such that

$$C_{f,r} = \sup_{g \in \mathcal{F}_{k^*}} \frac{\int |g - f|}{\int |\pi_r(g) - \pi_r(f)|} < \infty. \tag{5}$$

If $K_n = k^*$ then

$$\begin{aligned}
\int |\pi_r(\tilde{f}_{n,r}) - \pi_r(f)| &\leq \int |\pi_r(\tilde{f}_{n,r}) - \xi_{n,r}| + \int |\pi_r(f) - \xi_{n,r}| \\
&= \min_{g \in \mathcal{F}_{k^*}} \int |\pi_r(g) - \xi_{n,r}| + \int |\pi_r(f) - \xi_{n,r}| \\
&\leq \int |\pi_r(f) - \xi_{n,r}| + \int |\pi_r(f) - \xi_{n,r}|.
\end{aligned}$$

Therefore, by condition (5),

$$\begin{aligned}\int |\tilde{f}_{n,r} - f| &\leq C_{f,r} \int |\pi_r(\tilde{f}_{n,r}) - \pi_r(f)| \\ &\leq 2C_{f,r} \int |\pi_r(f) - \xi_{n,r}|.\end{aligned}$$

Using Theorem 1, it easily follows, under the additional condition that f has compact support (see Devroye and Györfi [6], Theorem 6, page 99), that

$$\mathbf{E}\left\{ \int |\tilde{f}_{n,r} - f| \right\} \leq 2C_{f,r}\mathbf{E}\left\{ \int |\pi_r(f) - \xi_{n,r}| \right\} \leq C_{f,r}\frac{\mathrm{C}}{\sqrt{nr^d}},$$

where C is a positive constant. Therefore, for such fixed r, we can have rate $\mathrm{O}(1/\sqrt{n})$. Unfortunately, condition (5) is hard to verify, and requires that the operator π_r is invertible on $\mathcal{F}_{k^*}$ and the inverse is continuous. We cannot handle our standard examples. However, for the class of normal densities, this condition holds for any fixed r. In other words, there is no need to choose small r, *i.e.*, the projection of non-consistent (asymptotically biased) histogram results in a good density estimate. ■

4 Proofs

From now on, all limits are taken as n goes to infinity.

4.1 Proof of Theorem 1

We split the proof into two steps in which bounds for $\mathbf{P}\{K_n > k^*\}$ (Step 1) and $\mathbf{P}\{K_n < k^*\}$ (Step 2) are obtained.

Step 1. Note that since f belongs to $\mathcal{F}_{k^*}$, one has

$$d_{n,k^*} \leq \sum_{A \in \mathcal{P}_n} \left| \int_A f - \mu_{2n}(A) \right| = \sum_{A \in \mathcal{P}_n} |\mu(A) - \mu_{2n}(A)|.$$

Consequently,

$$\begin{aligned}\{K_n > k^*\} &\subset \{d_{n,k^*} > T_n\} \\ &\subset \left\{ \sum_{A \in \mathcal{P}_n} |\mu(A) - \mu_{2n}(A)| > \sum_{A \in \mathcal{P}_n} |\mu_n(A) - \mu'_n(A)| \right\}.\end{aligned}$$

For $A \in \mathcal{P}_n$, set

$$I_n(A) = |\mu(A) - \mu_{2n}(A)| - |\mu_n(A) - \mu'_n(A)|,$$

and

$$\varepsilon_n = -\sum_{A \in \mathcal{P}_n} \mathbf{E}\left\{I_n(A)\right\}.$$

In the next paragraph, we prove that, for all n large enough,

$$\varepsilon_n \geq \frac{\kappa_1}{\sqrt{n h_n^d}}, \tag{6}$$

for some positive constant κ_1 depending on f. We can apply McDiarmid's inequality (cf. McDiarmid [12], see also Devroye, Györfi and Lugosi [7], Theorem 9.2, page 136). We have $2n$ random variables and the fluctuation of $\sum_{A \in \mathcal{P}_n} I_n(A)$ is at most $3/n$. Therefore

$$\begin{aligned}
\mathbf{P}\left\{K_n > k^*\right\} &\leq \mathbf{P}\left\{\sum_{A \in \mathcal{P}_n} I_n(A) > 0\right\} \\
&= \mathbf{P}\left\{\sum_{A \in \mathcal{P}_n} \left[I_n(A) - \mathbf{E}\left\{I_n(A)\right\}\right] > \varepsilon_n\right\} \\
&\leq \exp\left(-\frac{2\varepsilon_n^2}{2n(3/n)^2}\right) \\
&\leq \exp\left(-\frac{\kappa_1^2}{9} h_n^{-d}\right) \\
&= \exp\left(-\frac{\kappa_1^2}{9} n^{d\delta}\right).
\end{aligned}$$

Step 2. Denote by f_n (*resp.* f_{2n}) the standard histogram estimate drawn from the data $X_1, \ldots, X_n$ (*resp.* $X_1, \ldots, X_{2n}$) and the partition $\mathcal{P}_n$. That is, for $x \in \mathbb{R}^d$,

$$f_n(x) = \frac{\mu_n\left(A_n(x)\right)}{h_n^d} \quad \text{and} \quad f_{2n}(x) = \frac{\mu_{2n}\left(A_n(x)\right)}{h_n^d},$$

where $A_n(x)$ is the cell of the partition $\mathcal{P}_n$ containing x. For any density g, let $\pi_n(g)$ be defined by

$$\pi_n(g)(x) = \frac{1}{h_n^d} \int_{A_n(x)} g.$$

Clearly, for any g in $\mathcal{D}$, by the triangle inequality,

$$\begin{aligned} \sum_{A \in \mathcal{P}_n} \left| \int_A g - \mu_{2n}(A) \right| &= \int |\pi_n(g) - f_{2n}| \\ &\geq \int |\pi_n(g) - \pi_n(f)| - \int |\pi_n(f) - f_{2n}|. \end{aligned}$$

Therefore

$$\begin{aligned} \{K_n < k^*\} &\subset \{d_{n,k^*-1} \leq T_n\} \\ &\subset \left\{ \inf_{g \in \mathcal{F}_{k^*-1}} \int |\pi_n(g) - \pi_n(f)| \leq \int |\pi_n(f) - f_{2n}| + T_n \right\}. \end{aligned}$$

We shall prove that under the closure condition on the models $\mathcal{F}_k$, there exists $\Delta > 0$ satisfying

$$\liminf_{n \to \infty} \inf_{g \in \mathcal{F}_{k^*-1}} \int |\pi_n(g) - \pi_n(f)| = 3\Delta. \tag{7}$$

Then, because of

$$\begin{aligned} \mathbf{P}\{T_n \geq \Delta\} &\leq 2\mathbf{P} \left\{ \sum_{A \in \mathcal{P}_n} \left| \mu_n(A) - \int_A f \right| \geq \Delta/2 \right\} \\ &= 2\mathbf{P} \left\{ \int |f_n - \pi_n(f)| \geq \Delta/2 \right\}, \end{aligned}$$

we deduce that there exists a positive constant κ_2 depending on f such that, for all n large enough,

$$\begin{aligned} \mathbf{P}\left\{K_n < k^*\right\} &\leq 2\mathbf{P} \left\{ \int |f_n - \pi_n(f)| \geq \Delta/2 \right\} + \mathbf{P} \left\{ \int |\pi_n(f) - f_{2n}| \geq \Delta \right\} \\ &\leq 7 \exp(-\kappa_2 n). \end{aligned}$$

The last exponential inequality arises from Devroye and Györfi [6] (Lemma 4, page 22). Since $nh_n^d \to \infty$, it follows that, for all n large enough,

$$\begin{aligned} \mathbf{P}\left\{K_n < k^*\right\} &\leq 7 \exp(-\kappa_2 h_n^{-d}) \\ &= 7 \exp(-\kappa_2 n^{d\delta}). \end{aligned}$$

In order to prove (7) we use an indirect argument. Assume that

$$\liminf_{n\to\infty} \inf_{g\in\mathcal{F}_{k^*-1}} \int |\pi_n(g) - \pi_n(f)| = 0,$$

and, possibly extracting a subsequence, that

$$\lim_{n\to\infty} \inf_{g\in\mathcal{F}_{k^*-1}} \int |\pi_n(g) - \pi_n(f)| = 0.$$

By the Abou-Jaoude theorem, we obtain

$$\lim_{n\to\infty} \inf_{g\in\mathcal{F}_{k^*-1}} \int |\pi_n(g) - f| = 0.$$

Thus, if this is true, there exists a sequence (g_n) in $\mathcal{F}_{k^*-1}$ such that

$$\lim_{n\to\infty} \int |\pi_n(g_n) - f| = 0. \tag{8}$$

Observe now that for any bounded Lipschitz function φ on $\mathbb{R}^d$, the following chain of equalities is valid:

$$\begin{aligned}
\int \pi_n(g_n)\varphi &= \sum_{A\in\mathcal{P}_n} \int_A \frac{1}{h_n^d} \left(\int_A g_n\right) \varphi \\
&= \sum_{A\in\mathcal{P}_n} \int_A g_n \left(\frac{1}{h_n^d} \int_A \varphi\right) \\
&= \sum_{A\in\mathcal{P}_n} \int_A g_n \pi_n(\varphi) \\
&= \int g_n \pi_n(\varphi).
\end{aligned}$$

Moreover, as φ is Lipschitz, there exists a constant $c > 0$ such that, for all $n \geq 1$,

$$\sup_{\mathbb{R}^d} |\pi_n(\varphi) - \varphi| \leq c \sup_{A\in\mathcal{P}_n} \operatorname{diam} A,$$

and the right-hand term above goes to 0 because the partition $\mathcal{P}_n$ is cubic. Using the fact that g_n is a density function, and collecting the above results, we obtain

$$\lim_{n\to\infty} \left(\int \pi_n(g_n)\varphi - \int g_n\varphi\right) = 0.$$

Therefore, using (8) and the fact that φ is bounded, we are led to

$$\lim_{n\to\infty} \int g_n \varphi = \int f\varphi.$$

Since this equality holds for any bounded Lipschitz function, it also holds for any bounded and continuous function (see Dudley [10], Theorem 11.3.3, page 395). Invoking the closure of the class $\mathcal{F}_{k^*-1}$, we finally deduce that $f \in \mathcal{F}_{k^*-1}$, which is a contradiction. This proves equality (7). ■

4.2 Proof of (6)

By Jensen's inequality,

$$\begin{aligned}
\mathbf{E}\left\{|\mu_n(A) - \mu'_n(A)|\right\} &= \mathbf{E}\left\{\mathbf{E}\left\{|\mu_n(A) - \mu'_n(A)| \mid X_1, \ldots, X_n\right\}\right\} \\
&\geq \mathbf{E}\left\{|\mu_n(A) - \mathbf{E}\left\{\mu'_n(A) \mid X_1, \ldots, X_n\right\}|\right\} \\
&= \mathbf{E}\left\{|\mu_n(A) - \mu(A)|\right\}.
\end{aligned}$$

Therefore

$$\begin{aligned}
\varepsilon_n &= \sum_{A\in\mathcal{P}_n} \left[\mathbf{E}\left\{|\mu_n(A) - \mu'_n(A)|\right\} - \mathbf{E}\left\{|\mu_{2n}(A) - \mu(A)|\right\}\right] \\
&\geq \sum_{A\in\mathcal{P}_n} \left[\mathbf{E}\left\{|\mu_n(A) - \mu(A)|\right\} - \mathbf{E}\left\{|\mu_{2n}(A) - \mu(A)|\right\}\right] \\
&\triangleq \varepsilon'_n,
\end{aligned}$$

so instead of (6) it suffices to show that for some positive constant c_f and all n large enough,

$$\varepsilon'_n \geq \frac{c_f}{\sqrt{nh_n^d}}. \tag{9}$$

Let $B(n,p)$ denote a binomial random variable.

Lemma 1. *There exists a positive universal constant γ such that*

$$\left|\mathbf{E}\left\{|B(n,p) - np|\right\} - \sqrt{\frac{2np(1-p)}{\pi}}\right| \leq \gamma.$$

PROOF. Let Φ denote the standard normal distribution function, let F denote the distribution function of $B(n,p)$, let $m = np$ and $\sigma^2 = np(1-p)$. We will use the facts:

$$\mathbf{E}\left\{|B(n,p) - np|\right\} = \int_m^\infty (1 - F(x))\ \mathrm{d}x + \int_{-\infty}^m F(x)\ \mathrm{d}x$$

and

$$\left|\mathbf{P}\left\{B(n,p) \le m + x\sigma\right\} - \Phi(x)\right| \le \frac{Cn\mathbf{E}\left\{|B(1,p) - p|^3\right\}}{\sigma^3(1+|x|^3)} \tag{10}$$

by a local version of the Berry-Esseen inequality, where C is a positive universal constant (cf. Nagaev [13]). Working out (10), we note that

$$\mathbf{E}\left\{|B(1,p) - p|^3\right\} = p(1-p)^3 + (1-p)p^3 = p(1-p)((1-p)^2 + p^2) \le p(1-p).$$

Thus, the bound becomes

$$\frac{Cnp(1-p)}{(np(1-p))^{3/2}\,(1+|x|^3)} = \frac{C}{\sqrt{np(1-p)}(1+|x|^3)}. \tag{11}$$

Therefore

$$\begin{aligned}&\left|\int_m^\infty (1 - F(x))\ \mathrm{d}x - \int_m^\infty \left(1 - \Phi\left(\frac{x-m}{\sigma}\right)\right)\ \mathrm{d}x\right| \\ &\quad\le \int_m^\infty \frac{C}{\sqrt{np(1-p)}\left(1 + |(x-m)/\sigma|^3\right)}\ \mathrm{d}x\end{aligned}$$

by (11). After replacing $(x-m)/\sigma$ by y, we obtain

$$\left|\int_m^\infty (1 - F(x))\ \mathrm{d}x - \sigma\int_0^\infty (1 - \Phi(y))\ \mathrm{d}y\right| \le \int_0^\infty \frac{C}{1+|y|^3}\ \mathrm{d}y \stackrel{\triangle}{=} \gamma/2.$$

Thus,

$$\left|\int_m^\infty (1 - F(x))\ \mathrm{d}x - \frac{\sigma}{\sqrt{2\pi}}\right| \le \gamma/2.$$

Similarly,

$$\left|\int_{-\infty}^m F(x)\ \mathrm{d}x - \frac{\sigma}{\sqrt{2\pi}}\right| \le \gamma/2.$$

Finally,

$$\left|\mathbf{E}\left\{|B(n,p) - np|\right\} - \frac{2\sigma}{\sqrt{2\pi}}\right| \le \gamma.$$

■

Lemma 2.

$$\mathbf{E}\left\{|B(n,p)-np|\right\}-\frac{1}{2}\mathbf{E}\left\{|B(2n,p)-2np|\right\}\geq 0.$$

PROOF. If $B(n,p)$ and $B'(n,p)$ are i.i.d., then

$$B(2n,p)=B(n,p)+B'(n,p).$$

Thus,

$$\begin{aligned}\mathbf{E}\left\{|B(2n,p)-2np|\right\} &\leq \mathbf{E}\left\{|B(n,p)-np|\right\}+\mathbf{E}\left\{|B'(n,p)-np|\right\}\\ &= 2\mathbf{E}\left\{|B(n,p)-np|\right\}.\end{aligned}$$

■

Lemma 3.

$$\left|\mathbf{E}\left\{|B(n,p)-np|\right\}-\frac{1}{2}\mathbf{E}\left\{|B(2n,p)-2np|\right\}-\alpha\sqrt{np(1-p)}\right|\leq\frac{3\gamma}{2},$$

where

$$\alpha=\left(1-\frac{1}{\sqrt{2}}\right)\sqrt{\frac{2}{\pi}}.$$

PROOF. By Lemma 1, using ζ, ζ' for numbers in $[-\gamma,\gamma]$,

$$\begin{aligned}&\mathbf{E}\left\{|B(n,p)-np|\right\}-\frac{1}{2}\mathbf{E}\left\{|B(2n,p)-2np|\right\}\\ &=\sqrt{\frac{2np(1-p)}{\pi}}-\frac{1}{2}\sqrt{\frac{4np(1-p)}{\pi}}+\zeta+\zeta'/2\\ &=\left(1-\frac{1}{\sqrt{2}}\right)\sqrt{\frac{2np(1-p)}{\pi}}+\zeta+\zeta'/2.\end{aligned}$$

■

We are now in position to prove (6). To this aim, we show that under the conditions of Theorem 1,

$$\liminf_{n\to\infty}\sqrt{nh_n^d}\varepsilon_n'\geq\alpha\int\sqrt{f}.$$

Note that when the right-hand-side is infinite, inequality (9) is trivially true.

PROOF. Take $1/2 > \varepsilon > 0$ arbitrary. Because of the absolute continuity of μ and $h_n \to 0$,

$$\sup_{A \in \mathcal{P}_n} \mu(A) < \varepsilon$$

for all n large enough. Thus, by Lemma 2 and Lemma 3, we obtain

$$\begin{aligned}
\varepsilon_n' &= \sum_{A \in \mathcal{P}_n} \Big[\mathbf{E}\left\{ |\mu_n(A) - \mu(A)| \right\} - \mathbf{E}\left\{ |\mu_{2n}(A) - \mu(A)| \right\} \Big] \\
&= \frac{1}{n} \sum_{A \in \mathcal{P}_n} \left[\mathbf{E}\left\{ |B(n, \mu(A)) - n\mu(A)| \right\} - \frac{1}{2} \mathbf{E}\left\{ |B(2n, \mu(A)) - 2n\mu(A)| \right\} \right] \\
&\geq \frac{1}{n} \sum_{A \in \mathcal{P}_n} \left[\alpha \sqrt{n\mu(A)\left((1 - \mu(A)\right)} - \frac{3\gamma}{2} \right]^+ \\
&\geq \frac{1}{n} \sum_{A \in \mathcal{P}_n} \left[\alpha \sqrt{1 - \varepsilon} \sqrt{n\mu(A)} - \frac{3\gamma}{2} \right]^+ \\
&\geq \frac{1}{n} \sum_{A \in \mathcal{P}_n,\, \sqrt{n\mu(A)} \geq \beta} \alpha (1 - \varepsilon)^{3/2} \sqrt{n\mu(A)} \\
&= \frac{\alpha (1 - \varepsilon)^{3/2}}{\sqrt{n}} \sum_{A \in \mathcal{P}_n, \sqrt{n\mu(A)} \geq \beta} \sqrt{\mu(A)},
\end{aligned}$$

where

$$\beta = \frac{3\gamma}{2\alpha\varepsilon\sqrt{1 - \varepsilon}}.$$

Thus, by Jensen's inequality,

$$\begin{aligned}
\sqrt{nh_n^d}\varepsilon_n' &\geq \alpha (1 - \varepsilon)^{3/2} \sum_{A \in \mathcal{P}_n,\, \sqrt{n\mu(A)} \geq \beta} \sqrt{h_n^d \mu(A)} \\
&= \alpha (1 - \varepsilon)^{3/2} \sum_{A \in \mathcal{P}_n,\, \sqrt{n\mu(A)} \geq \beta} \sqrt{h_n^d \int_A f(x)\, \mathrm{d}x} \\
&\geq \alpha (1 - \varepsilon)^{3/2} \sum_{A \in \mathcal{P}_n,\, \sqrt{n\mu(A)} \geq \beta} \int_A \sqrt{f(x)}\, \mathrm{d}x \\
&= \alpha (1 - \varepsilon)^{3/2} \int \sqrt{f(x)}\, \mathbf{1}_{\{\sqrt{n\mu(A_n(x))} \geq \beta\}}\, \mathrm{d}x.
\end{aligned}$$

By Fatou's lemma,

$$\begin{aligned}\liminf_{n\to\infty}\sqrt{nh_n^d}\varepsilon_n' &\geq \alpha(1-\varepsilon)^{3/2}\int\sqrt{f(x)}\liminf_{n\to\infty}\mathbf{1}_{\{\sqrt{n\mu(A_n(x))}\geq\beta\}}\,\mathrm{d}x\\ &\geq \alpha(1-\varepsilon)^{3/2}\int_{\{x:f(x)>0\}}\sqrt{f(x)}\liminf_{n\to\infty}\mathbf{1}_{\{\sqrt{n\mu(A_n(x))}\geq\beta\}}\,\mathrm{d}x.\end{aligned}$$

By the Lebesgue density theorem, for almost all x, $\mu\left(A_n(x)\right)/h_n^d \approx f(x)$, therefore the condition $nh_n^d \to \infty$ implies that for almost all x satisfying $f(x) > 0$, and for any β,

$$\liminf_{n\to\infty}\mathbf{1}_{\{\sqrt{n\mu(A_n(x))}\geq\beta\}} = \liminf_{n\to\infty}\mathbf{1}_{\left\{\sqrt{nh_n^d\frac{\mu(A_n(x))}{h_n^d}}\geq\beta\right\}} = 1.$$

Thus,

$$\liminf_{n\to\infty}\sqrt{nh_n^d}\varepsilon_n' \geq \alpha(1-\varepsilon)^{3/2}\int\sqrt{f(x)}\,\mathrm{d}x.$$

As $\varepsilon > 0$ is arbitrary, (9) follows. ■

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References

[1] Biau, G. and Devroye, L. (2004). A note on density model size testing, *IEEE Transactions on Information Theory*, Vol. 50, pp. 576–581.

[2] Biau, G. and Devroye, L. (2005). Density estimation by the penalized combinatorial method, *Journal of Multivariate Analysis*, Vol. 94, pp. 196–208.

[3] Biau, G. and Györfi, L. (2005). On the asymptotic properties of a nonparametric L_1-test of homogeneity, *IEEE Transactions on Information Theory*, Vol. 51, pp. 3965–3973.

[4] Cao, R. and Lugosi, G. (2005). Goodness-of-fit tests based on the kernel density estimator, *Scandinavian Journal of Statistics*, Vol. 32, pp. 599–616.

[5] Devroye, L. (1997). Universal smoothing factor selection in density estimation: Theory and practice (with discussion), *Test*, Vol. 6, pp. 223-320.

[6] Devroye, L. and Györfi, L. (1985). *Nonparametric Density Estimation: The L_1 View*, Wiley, New York.

[7] Devroye, L., Györfi, L. and Lugosi, G. (1996). *A Probabilistic Theory of Pattern Recognition*, Springer–Verlag, New York.

[8] Devroye, L. and Lugosi, G. (2001). *Combinatorial Methods in Density Estimation*, Springer–Verlag, New York.

[9] Dudley, R.M. (1978). Central limit theorems for empirical measures, *The Annals of Probability*, Vol. 6, pp. 899–929.

[10] Dudley, R.M. (2002). *Real Analysis and Probability*, Cambridge University Press, Cambridge.

[11] James, L.F., Priebe, C.E. and Marchette, D.J. (2001). Consistent estimation of mixture complexity, *The Annals of Statistics*, Vol. 29, pp. 1281–1296.

[12] McDiarmid, C. (1989). On the method of bounded differences, in *Surveys in Combinatorics 1989*, pp. 148–188, Cambridge University Press, Cambridge.

[13] Nagaev, S.V. (1965). Some limit theorems for large deviations (Russian), *Teor. Verojatnost. i Primenen*, Vol. 10, pp. 231–254.

[14] Priebe, C.E. (1994). Adaptive mixtures, *Journal of the American Statistical Association*, Vol. 89, pp. 796–806.

[15] Rogers, G.W., Marchette, D.J. and Priebe, C.E. (2002). A procedure for model complexity selection in semiparametric mixture model density estimation, *Technical Report*, Naval Surface Warfare Center, Dahlgren Division, Virginia.

[16] Vapnik, V.N. and Chervonenkis, A.Ya. (1971). On the uniform convergence of relative frequencies of events to their probabilities, *Theory of Probability and its Applications*, Vol. 16, pp. 264–280.

[17] Yatracos, Y.G. (1985). Rates of convergence of minimum distance estimators and Kolmogorov's entropy, *The Annals of Statistics*, Vol. 13, pp. 768–774.